

November 15, 2001

Walter L. Jones
Pine Chemicals Association
P.O. Box 105113
Atlanta, GA 30348-5113

Dear Mr. Jones:

The Office of Pollution Prevention and Toxics is transmitting EPA's comments on the robust summaries and test plan for "Tall Oil Fatty Acids and Related Substances", posted on the ChemRTK Web site on June 14, 2001. I commend The Pine Chemicals Association for its commitment to the HPV Challenge Program.

EPA reviews test plans and robust summaries to determine whether the reported data and test plans will provide the data necessary to adequately characterize each SIDS endpoint. On its Chemical RTK HPV Challenge Program web site EPA has provided guidance for determining the adequacy of data and preparing test plans used to prioritize chemicals for further work.

EPA has a number of comments on the submission; see the enclosure for details. While the category approach is on the whole reasonable, the Association has not adequately discussed and justified the substantial differences in composition among certain category members nor shown how the test results for tall oil fatty acid would apply to the characterization of monomer acid and branched and linear octadecanoic acid, category members that typically comprise about 50% of substances not found in the other members.

Though the Test Plan indicated that there is no need to measure vapor pressure, photodegradation and transport and distribution for these chemicals, EPA believes that there should be measured vapor pressure data and estimated photodegradation and transport/distribution data for the major constituents (see Test Plan comments).

For ecological effects, EPA agrees with the category rationale, but recommends 21-day chronic toxicity testing for daphnid rather than acute tests. All aquatic testing should follow the guidelines for hydrophobic substances and poorly water-soluble chemicals.

As with other submissions where the available data are either inadequate or insufficiently documented, this case will remain open until adequate documentation is in hand.

EPA will post this letter and the attached Comments on the Chemical RTK web site within the next few days. As noted in the comments, we ask that the Association advise the Agency, within 60 days of the posting on the Chemical RTK website, of any modifications to its submission.

As mentioned in our November 2, 2000, letter to PCA, EPA expects that the data developed under the HPV Challenge Program on monomer acid (now correctly named Fatty acids, C16-18 and C18-unsatd., branched and linear)(CAS No. 68955-98-6) and related substances will satisfy Agency information needs for any new PMNs submitted as a result of the June 27, 2001 (66 FR 34193) FR Notice "Correction to Chemical Nomenclature for Monomer Acid and Derivatives for TSCA Inventory Purpose."

If you have any questions about this response, please contact Richard Hefter, Chief of the HPV Chemicals Branch, at 202-564-7649. Submit general questions about the HPV Challenge Program through the Chemical RTK web site comment button or through the TSCA Assistance Information Service (TSCA Hotline) at (202) 554-1404. The TSCA Hotline can also be reached by e-mail at tsc-hotline@epa.gov.

I thank you for your submission and look forward to your continued participation in the HPV Challenge Program.

Sincerely,

/s/

Oscar Hernandez, Director
Risk Assessment Division

Enclosure

cc: W. Sanders
A. Abramson
C. Auer
M. E. Weber

EPA Comments on Chemical RTK HPV Challenge Submission: Tall Oil Fatty Acids and Related Substances

SUMMARY OF EPA COMMENTS

The sponsor, the Pine Chemicals Association, Inc. submitted a Test Plan and Robust Summaries to EPA dated May 31, 2001, for the Tall Oil Fatty Acids and Related Substances Category. EPA posted the submission on the ChemRTK HPV Challenge Web site on June 14, 2001. The proposed information-gathering plan is for six substances and mixtures (see Category Definition, below) considered by the sponsor to constitute a category.

EPA has reviewed this submission and has reached the following conclusions:

1. The category approach is on the whole reasonable on the basis of structure, physicochemical properties, and health effects (see Category Justification). However, the submitter has not adequately discussed and justified the differences in composition for certain category members.
2. Physicochemical and Environmental Fate Data. The submitter indicated in its Test Plan that there is no need to measure vapor pressure, photodegradation and transport and distribution for these chemicals. EPA believes that the submitter should provide measured vapor pressure data and estimated photodegradation and transport/distribution data for the major constituents of these chemicals (see Test Plan comments below).
3. Health Endpoints: The available mammalian toxicity testing was done on tall oil fatty acid. Although these data address nearly all the required SIDS-level health effects endpoints, they may not adequately characterize the toxicity of monomer acid or branched and linear octadecanoic acid, category members that typically contain about 25% branched acids and 25% C₁₈ acids of unknown structure ("probably cyclic"). The submitter needs to explain how the test results for tall oil fatty acid would apply to the characterization of monomer acid and branched and linear octadecanoic acid.
4. Ecological effects. EPA agrees with the submitter's rationale for the category definition and justification, but recommends 21-day chronic toxicity testing for daphnid rather than acute tests. All aquatic testing should follow the guidelines for hydrophobic substances and poorly water-soluble chemicals in the Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures (OECD, June 2000 – available on the OECD website at <http://www.oecd.org/ehs/test/monos.htm>).

EPA requests that the Submitter advise the Agency within 60 days of any modifications to its submission.

EPA COMMENTS ON THE TALL OIL FATTY ACIDS AND RELATED SUBSTANCES CHALLENGE SUBMISSION

Category Definition

The proposed information-gathering plan is for six mixtures: low boiling tall oil fatty acid (CAS No. 65997-03-7), tall oil fatty acid (CAS No. 61790-12-3) and its sodium and potassium salts (CAS No. 61790-45-2 and 61790-44-1), branched and linear C16-C18 and C18 unsaturated fatty acids (monomer acid, CAS No. 68955-98-6), and branched and linear octadecanoic acid (CAS No. 68201-37-6).

Except for incomplete identification of the latter two substances (see Category Justification, below), the category definition is clear.

Category Justification

The category justification is primarily based on the composition of the category members, which predominantly contain C₁₈ unsaturated and saturated fatty acids and salts. The salts are included in the category because they are “. . . quickly converted into the free acids when they are neutralized by acid or by dilution, as they would be under typical toxicity testing conditions.” However, the typical compositions cited for the monomer acid and branched and linear octadecanoic acid members show 24% C₁₈ “probably cyclic” acids of unknown structure and 28% of branched C₁₈ acids that are significantly different from the tall oil fatty acid constituents. Similarly, there is a significant difference in the quantity of “unsaponifiable matter” between tall oil heads (10%) and tall oil fatty acids (1%). The unsaponifiable matter includes various terpenic hydrocarbon, alcohols, aldehydes, phenolics, lignin-derived materials, and other neutral materials. Given that 50% of the compositions of two category members differ from the other four, the submitter needs to discuss specifically the compositional differences in the category members and justify including them in a single category.

Although not stated, it appears that the branched and “probably cyclic” constituents cited above arise in the processing of tall oil fatty acid to other products. It would be helpful for the submitter to confirm this.

Test Plan

Representative Test Substance

The submitter bases the selection of tall oil fatty acid as the test substance on its high production volume and the fact that four of the six category members are derived from tall oil fatty acids and “are similar in chemical composition.” However, about 50% of the compositions of two category members differ from the other four (see Category Justification, above). It is unclear what effect the differences in composition will have on toxicity. Available toxicity data suggest that tall oil fatty acids have very low toxicity and it is possible that the other members of the category have similar toxicity. Nonetheless, there was no discussion acknowledging the differences in the category members and explaining why the use of tall oil fatty acids as the test material would support reading across to the toxicity of the other members. A discussion with this focus would allow a better understanding of the category and permit an informed assessment of the testing strategy.

Chemistry (melting point, boiling point, vapor pressure, water solubility, and partition coefficient)

The sponsor’s approach for melting point, boiling point, Log P, and water solubility is acceptable for the purposes of the U.S. HPV Challenge Program

Vapor Pressure

The submitter states on page 14 of the Test Plan that: “Vapor Pressures for the fatty acids at ambient temperatures are effectively zero, and their experimental measurement is inappropriate.” EPA believes that vapor pressures should be measured for the most volatile fatty acid components, or at least for the major constituents of these chemicals (which the submitter identifies on pages 9 and 10 of its Test Plan – oleic acid, linoleic acid, palmitic acid, elaidic acid, etc.). EPA agrees with the submitter that the vapor pressure for the salts in this category can be considered negligible for the purpose of evaluating their environmental fate.

Environmental Fate (Photodegradation, Stability in Water, Biodegradation, Fugacity)

The submitter’s approach for water stability and biodegradation is acceptable for the purposes of the HPV Challenge Program.

Photodegradation

The submitter indicates on page 16 of its Test Plan that: "Due to their low water solubility and lack of any vapor pressure, there is no opportunity for any of these chemicals to enter the atmosphere. Thus, photodegradation is irrelevant." EPA believes that photodegradation should be measured for the major constituents of these chemicals because their Henry's Law constants suggest that these chemicals may volatilize and degrade by reaction in the atmosphere with photochemically formed hydroxyl radicals.

Transport and Distribution (Fugacity)

The submitter provides no transport and distribution data. EPA believes that transport and distribution data should be estimated for the major constituents of these chemicals. EPA recommends using the EQC Level III model, which is more realistic and useful for estimating a chemical's fate in the environment. In order to develop the Level III fugacity model, EPA recommends using the EQC Level III model from the Canadian Environment Modeling Centre at Trent University, which allows full control of data inputs. This model can be found at the following web address: <http://www.trentu.ca/academic/aminss/envmodel>

Health Effects (acute toxicity, repeat dose toxicity, genetic toxicity, and reproductive/developmental toxicity).

The data for tall oil fatty acids indicate a low order of toxicity and adequately characterize the toxicity of the other members of this category except for the two members that contain cyclic acids of unknown structure. It is unlikely that the variations in composition described in the test plan would substantially alter the toxicity of the members of this category. However, because these cyclic acids apparently are not present in tall oil fatty acid, they could impart toxicologic properties that could not be anticipated from the observed toxicity studies of tall oil fatty acid. A better understanding of the specific chemicals that make up the unknown "probably cyclic" acids, and of how they arise, would help confirm that their toxicologic properties resemble those of the other chemicals in these complex mixtures.

Genetic Toxicity Data: EPA agrees with the proposed testing for genotoxicity in an in vitro mammalian chromosome aberration test (OECD Guideline 473), both with and without metabolic activation.

Ecotoxicity

EPA disagrees with the proposed acute toxicity testing of fish, daphnia, and algae. Rather, EPA recommends the daphnid reproduction 21-day chronic test using a flow-through method with measured concentrations. High log Kow chemicals having an anionic group may not be able to achieve optimal aquatic effects in short-term tests. EPA further recommends that the water solubility test should be performed at pH7 and prior to the toxicity test. The tall oil fatty acids should then be tested for environmental toxicity up to their dispersible limits as the sodium salt, at pH 7, at 25°C, and a dilution water hardness of less than 180 mg/L as CaCO₃. No dispersants should be used owing to possible interference with inherent toxicity of test chemicals. Also, EPA agrees with the submitter's proposal to test chemicals under conditions that maximize solubility but reduce exposure to insoluble fractions that may cause nonspecific toxicological effects. EPA cautions that these conditions should incorporate approved analytical methods and should follow the Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures (OECD, June 2000—available on the OECD website at <http://www.oecd.org/ehs/test/monos.htm>).

SPECIFIC COMMENTS ON ROBUST SUMMARIES

Health Effects Studies

Repeated-Dose Toxicity. Among the two studies submitted, only the 90-day repeated-dose toxicity study summary is adequate. The 28-day study is inadequate and has the following deficiencies: only males were tested, no data were collected for hematology, clinical chemistry or histopathology. In addition, the study summary has an incorrect CAS number for tall oil fatty acid "51790-12-3" instead of "61790-12-3."

Followup Activity

EPA requests that the Submitter advise the Agency within 60 days of any modifications to its submission.